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Laboratory Astrophysics under the Ultraviolet, Visible, and Gravitational Astrophysics Research Program

Final Technical Report for Grant NAGW-3840 Oscillator Strengths for Ultraviolet Atomic Transitions

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I. Introduction

Space-borne facilities, such as the *Hubble Space Telescope*, the recent ORFEUS-SPAS II Shuttle mission, and the soon-to-be launched *Far Ultraviolet Spectroscopic Expolorer*, are providing data at ultraviolet wavelengths of unprecedented quality for spectroscopic studies of many astronomical environments. The first step in the analysis of these data involves the derivation of abundances. Obtaining accurate abundances is possible only when the correspondence between line strength and abundance is well known. The conversion of line strength to abundance relies on knowledge of mean lives and oscillator strengths. For many ultraviolet transitions, the necessary atomic and molecular data are either relatively imprecise or not available. Our program addresses this need for accurate oscillator strengths; our focus is on transitions that probe the nature and composition of the interstellar medium.

II. Laboratory Results

During the reporting period two experimental methods were employed to extract oscillator strengths. Beam-foil spectroscopic techniques were used to measure mean lives and branching fractions for atomic transitions at ultraviolet wavelengths. An ion beam of the desired element was accelerated and passed through a thin carbon foil, where neutralization, ionization, and excitation take place. Mean lives were determined by measuring the decay of the excited state as a function of distance from the foil. Oscillator strengths were obtained from the mean life and branching fraction. The second technique involved absorption spectroscopy, where a gas cell containing the species of interest is placed in front of a source of ultraviolet radiation, such as a synchrotron. The measured absorption profiles were fitted to a theoretical profile to yield the amount of absorption from which the oscillator strength can be derived.

(i) Si II

Recent observations with the *Hubble Space Telescope* by Spitzer and Fitzpatrick (1993) suggested an f-value for λ 1526 that was within 20% of that calculated by Hibbert et al. (1992), rather than the value recommended by Morton (1991) which was based on previous astronomical observations of Shull et al. (1981). The principal previous experimental result, the phase-shift measurement of Curtis and Smith (1974), does not agree well either with the value recommended by Morton (1991) or with the very different value calculated by Hibbert et al. (1992). We, therefore, carried out a detailed beam-foil study of the Si II multiplet containing λ 1526.

Two independent measurements of the lifetime of the $3s^2$ 4s $^2S_{1/2}$ upper level were obtained. Cascade repopulation occurred relatively slowly and weakly, and multiple-exponential curve fitting could be used to extract a reliable mean life of 0.89 ± 0.04 ns. An ANDC measurement was also performed by recording decay curves for the cascading transition from the $3s^2$ 4p $^2P_{1/2}^{\circ}$ level through its decay to the 3s $3p^2$ 2D levels at 3862.6 Å. This resulted in a similar value for the mean life of 0.90 ± 0.06 ns. The total transition probability out of the $3s^2$ 4s $^2S_{1/2}$ level is the sum of the A-values to the two fine structure levels $3s^2$ $3p^2P_{1/2,3/2}^{\circ}$. Individual A-values for the components of the multiplet can be determined if the branching ratio of these two transitions is determined. According to LS coupling, the ratio of these two lines strengths should be 0.5, a prediction in reasonable agreement with the measurement of Hofmann (1969) of 0.49 ± 0.01 and with our somewhat poorer accuracy relative intensity measurement of 0.48 ± 0.02 . Using a weighted mean of the two experimental determinations to obtain individual A-values from the measured lifetime, a multiplet f-value of 0.130 ± 0.005 was obtained. This result is in excellent agreement with the early calculation of Weiss (1969) and the more recent calculations of Hibbert et al. (1992), both of whom obtained 0.130. The f-value for this multiplet is now firmly established and may be used with confidence in future observations.

The interstellar line at 1023 Å, arising from transitions to the $3s^2$ 5s 2S $_{1/2}$ level, may also be employed in interstellar studies. Here too, agreement between the previous experimental measurement (Curtis and Smith 1974) and theory (Weiss 1969; Hibbert et al. 1992) was only fair. We performed a beam-foil measurement of the mean life of the $3s^2$ 5s 2S $_{1/2}$ level and obtained the value 1.99 \pm 0.12 ns. This result is in good agreement with the early calculation of Weiss (1969), and it agrees with the theoretical calculation of Hibbert et al. (1992) to within 20%. Nevertheless, the results still differ by four experimental standard deviations. In a recent private communication, Hibbert (1996) noted that the disagreement between the length and velocity forms of the calculation suggests convergence — especially for the 4p-5s transition — had not been obtained in his previous calculation. Additional configurations would need to have been included to obtain a 5s lifetime with the same precision as reported for the 4s lifetime. Such calculations have not yet been performed, so that a more precise test of theory awaits the conclusion of the more complete calculation. A paper describing our Si II measurements has been prepared and is about to be submitted to *The Astrophysical Journal*.

Three graduate students, Murray Henderson, Henry Povolny, and David Knauth, worked on this project at various times with partial support from this grant. Murray now serves as the accelerator technician for the Department of Physics and Astronomy. Both Henry and David are continuing graduate study aimed at the Ph.D. degree.

Carbon monoxide is the second most abundant molecule in interstellar space. Ultraviolet data obtained with the Goddard High Resolution Spectrograph on the the *Hubble Space Telescope* yield high-quality spectra of the $A^{-1}\Pi - X^{-1}\Sigma^{+}$ (v',0) system of bands (e.g., Lambert et al. 1994). In order to extract the most reliable abundances, one is interested in the data for the weakest, optically thin bands, those with $v' \geq 7$. Unfortunately, the available theoretical and experimental data on oscillator strengths for these bands span a range of 20 - 30%, which is larger than the uncertainties associated with the astronomical measurements. In particular, an absorption experiment conducted at a synchrotron radiation source (Eidelsberg et al. 1992) reported results that are consistently 20 - 30% larger than the others. Since all results for bands with $v' \leq 6$ agree at the 5 - 10% level, the cause for the differences involving weaker bands is difficult to ascertain. As noted by Lambert et al. (1994), the differences in relative f-values between strong ($v' \leq 6$, 0) and weak bands ($v' \geq 7$, 0) from the molecular data available at the time compromise interstellar studies of chemical fractionation between different isotopic variants of CO. (The strong bands are used to derive the abundance of rare forms of CO in interstellar clouds, while the weak bands are needed for $^{12}C^{16}O$.) We conducted an experiment at the Synchrotron Radiation Center of the University of Wisconsin-Madison in an attempt to understand these differences in oscillator strength.

Federman et al. (1997) obtained f-values for the electronic transitions $A^{-1}\Pi - X^{-1}\Sigma^{+}$ (ν' , 0) where $\nu' = 7$, 8, 9, 10, 11 relative to the accurately known f-value for $A^{-1}\Pi - X^{-1}\Sigma^{+}$ (5, 0). Special care was taken in obtaining and analyzing the data. The gas cell containing the CO was very short, and at the pressures used in the experiment (30 to 1000 mTorr) resulted in columns of CO comparable to those derived for interstellar clouds by Lambert et al. (1994). This minimized the problem of analyzing optically thick lines, as did working at room temperature because the absorption was spread over many lines. Federman et al. (1997) fitted the observed bands with synthetic spectra in which they varied the excitation temperature and f-value in a least-squares manner until the rms deviation between observed and synthesized spectra was minimized. The column of CO needed for the synthesis was determined by fitting the measurements for the (5, 0) band whose f-value is accurately known.

Our relative oscillator strengths agree reasonably well with results from electron-impact excitation (Lassettre and Skerbele 1971; Chan et al. 1993) and theory (Kirby and Cooper 1989), but differ substantially from the results of the earlier absorption experiment (Eidelsberg et al. 1992). The extrapolation to zero pressure by Eidelsberg et al. (1992) may have been in error. The excellent agreement that now exists among the various techniques provides the basis for more secure astronomical studies. As a result of the success in this project, we are now considering similar measurements on other electronic transitions in the spectrum of CO.

III. Astronomical Results

(i) C I

As noted by Morton (1991), experimental and theoretical results are available for many C I transitions whose wavelengths are longward of 1200 Å. For dipole-allowed transitions in this range, there is good agreement among results. For weak transitions involving a change of spin, the comparisons are less satisfactory. de Boer and Morton (1974; 1979) and Jenkins et al. (1983) utilized interstellar spectra acquired with the *Copernicus* satellite to enlarge the database, with particular attention given to lines shortward of 1200 Å as well as to the stronger transitions where the spin is changed. Morton's (1991) compilation incorporates these astronomically derived f-values. The precision with which absorption lines can be measured off HST spectra, however, reveals inconsistencies when applying the f-values recommended by Morton (1991).

Zsargó, Federman, and Cardelli (1997) used HST data for the sight lines toward β^1 Sco, ρ Oph A, and χ Oph and obtained a self-consistent set of f-values, accurate to 10-20%, for lines shortward of 1200 Å and for lines arising from weak, spin-changing transitions. Much like the earlier studies with the *Copernicus* satellite noted above and the work on S I from HST spectra reported last time (Federman and Cardelli 1995), Zsargó et al. (1997) derived the column density and b-values for each fine structure level in the ground state from lines whose oscillator strengths have precise experimental values. In particular, their analysis was based on lines in the multiplets at 1261, 1277, 1280, and 1329 Å. The f-values for the other lines seen in the HST spectra were adjusted in a least-squares fashion until all lines gave the same column density and b-value for a given fine structure level. In all, they suggested refinements for about 50% of the lines detected in their interstellar spectra.

An interesting conclusion from the work of Zsargó et al. (1997) is that their f-values for individual lines within a multiplet do not obey LS coupling rules in several instances. The conclusion has important ramifications because line oscillator strengths from large-scale computations are usually derived from multiplet f-values through the use of LS coupling. If this approximation is not valid, the abundances obtained from these line oscillator strengths are not reliable. Zsargó et al. checked the validity of their finding through large-scale calculations based on the HFR formalism (Hartree-Fock plus lowest order relativistic corrections); the well-known code of Cowan (1981) with 16 configurations was used in this study. (This code is especially useful in searching for transitions where configuration interaction and spin-orbit mixing affect relative line strengths.) The theoretical predictions confirmed in a qualitative manner that while LS coupling is valid for the multiplets $\lambda\lambda$ 1157, 1193, line strengths for the multiplets $\lambda\lambda$ 1156, 1189, and 1194 do not follow LS coupling rules. Furthermore, the computation revealed the perturbing levels leading to configuration interaction and spin-orbit mixing in the latter cases. The refined oscillator strengths are now being applied to other HST data in our continuing efforts to study the interstellar medium.

Measurements of Ni II absorption from low density, warm material and higher density, cold diffuse gas (Sembach and Savage 1996) show that the largest range in depletion onto interstellar dust for these environments occurs for nickel. Thus, Ni II absorption in damped Ly- α systems is used to place constraints on the evolution of dust within the intervening galaxy over Hubble time scales (e.g., Prochaska and Wolfe 1996; 1997). Current analyses of Ni II abundance in interstellar environments rely on the oscillator strengths compiled by Morton (1991). These f-values come from the unpublished theoretical work of Kurucz (1989). Many of the lines listed by Morton (1991) appear in HST spectra of ρ Oph A, χ Oph, and ζ Oph. Zsargó and Federman (1997) analyzed these high-quality measurements so that an accurate set of relative f-values is available for future studies. Unlike the situations for S I (Federman and Cardelli 1995) and C I (Zsargó et al. 1997), the actual abundance for Ni II cannot yet be derived because laboratory f-values are not available for the lines covered by our observations. Zsargó and Federman found good agreement with the predictions of Kurucz (1989) for the strongest lines in their sample. For the three weakest lines, $\lambda\lambda$ 1345, 1415, and 1477, there are significant differences, however, ranging from 40% to 100%. Such differences are not unexpected for such a complicated atom. The work on C I and Ni II formed the basis of a Masters Thesis by Janos Zsargó, who is now pursuing a Ph. D. at the University of Toledo. We are performing experiments, in collaboration with Jim Lawler at the University of Wisconsin-Madison so that our relative oscillator strengths can be placed on an absolute scale.

IV. Conferences

The review talk given by Federman at the 5th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas has appeared in print (Federman and Cardelli 1996). Federman and Zsargó described the work on C I and Ni II as posters at the American Astronomical Meeting during June, 1996 in Madison, WI (Zsargó and Federman 1996) and at the conference The Scientific Impact of the Goddard High Resolution Spectrograph which was held at the Goddard Space Flight Center in September of 1997. They also presented their findings, including those on S I, at the ICAMDATA Conference held at the National Institute of Science and Technology in Gaithersburg, MD during October, 1997. Schectman and colleagues (Povolny et al. 1996) presented a poster on the Si II work at the meeting of the Division of Atomic, Molecular, and Optical Physics of the American Physical Society. This meeting took place in Ann Arbor, MI during May of 1996.

V. References

Bergeson, S.D., and Lawler, J.E. 1993, Ap. J. (Letters), 414, L137. Chan, W.F., Cooper, G., and Brion, C.E. 1993, Chem. Phys., 170, 123. Cowan, R.D. 1981, The Theory of Atomic Structure and Spectra, [Univ. California Press: Berkeley]. Curtis, L.J., and Smith, W.H. 1974, Phys. Rev., A9, 1537. de Boer, K.S., and Morton, D.C. 1974, Astron. Ap., 37, 305. _1979, Astron. Ap., 71, 141. Eidelsberg, M., Rostas, F. Breton, J., and Thieblemont, B. 1992, J. Chem. Phys., 96, 5585. Federman, S.R., and Cardelli, J.A. 1995, Ap. J., 452, 269. _1996, Physica Scripta, T65, 158. Federman, S.R., Menningen, K.L., Lee, W., and Stoll, J.B. 1997, Ap. J. (Letters), 477, L61. Hibbert, A. 1996, private communication. Hibbert, A., Ojha, P.C., and Stafford, R.P. 1992, J. Phys. B, 25, 4153. Hofmann, W. 1969, Z. Naturforsch., A24, 990. Jenkins, E.B., Jura, M., and Loewenstein, M. 1983, Ap. J., 270, 88. Kirby, K., and Cooper, D.L. 1989, J. Chem. Phys., 90, 4895. Kurucz, R.L. 1989, computer tapes. Lambert, D.L., Sheffer, Y, Gilliland, R.L., and Federman, S.R. 1994, Ap. J., 420, 756. Lassettre, E.N., and Skerbele, A., J. Chem. Phys. 1971, 54, 1597. Morton, D.C. 1991, Ap. J. Suppl., 77, 119. Povolny, H.S., Schectman, R.M., and Curtis, L.J. 1996, Bull. A.P.S., 41, 1146. Prochaska, J.X., and Wolfe, A.M. 1996, Ap. J., 470, 403. _1997, Ap. J., 474, 140.

_____1997, ApJ, in press. Zsargó, J., Federman, S.R., and Cardelli, J.A. 1997, Ap J., 484, 820.

Weiss, A. 1969, in Atomic Transition Probabilities 7 (NSRDS-NBS-22).

Sembach, K.R., and Savage, B.D. 1996, Ap. J., 457, 211. Shull, J.M., Snow, T.P., and York, D.G. 1981, Ap. J., 246, 549. Spitzer, L., and Fitzpatrick, E.L. 1993, Ap J., 409, 299.

Zsargó, J., and Federman, S.R. 1996, B.A.A.S., 28, 891.